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CRYSTAL PLASTICITY MODELLING OF MONOTONIC SHEAR TESTS ON PURE TITANIUM

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Summary: This study consists in the modelling of shear tests performed on pure titanium using a polycrystalline model. Numerical and experimental results are presented.

1 INTRODUCTION

The MULTISITE model [1] is based on polycrystalline plasticity and the underlying hypotheses of the model are (i) that the deformation of each grain is significantly influenced by the interaction with a limited number of adjacent grains, and (ii) that local strains deviate from their macroscopic average according to specific “relaxation modes”. The LAMEL model [2] is reformulated into the more general elastic-viscoplastic MULTISITE model permitting various relaxation modes. The model was used to simulate simple shear tests along different directions performed on high purity α-Titanium. The predicted texture and the mechanical behaviour are compared to experimental results.

2 NUMERICAL MODEL

The deformation textures predicted by the classical relaxed-constraints models are not really much better than those predicted by the full-constraints Taylor model. The suspected reason could be that the local interaction between adjacent grains is not taken into account. This statement led to develop the multi-grain models, specially the Lamel model.

The concept of “cluster of interaction” appears in the multi grain models. For comparison, in the Taylor model and the classical relaxed-constraints models, the cluster of interaction would contain only one grain; they are one-grain models with no interaction between adjacent grains. The multi-grain models use the same relaxation tensors as in the classical relaxed-constraints theories but they assume that the macroscopic velocity gradient is achieved collectively by the cluster of interacting grains. For instance, in the Lamel model (two-grains model), if the grain I interacts with the grain II, it implies that $\left(\underline{\underline{L}}^{micro,I} + \underline{\underline{L}}^{micro,II}\right)/2 = \underline{\underline{L}}^{macro}$.

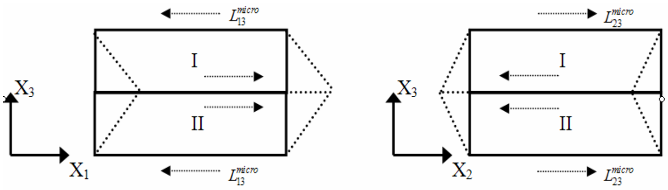

Figure 1: Relaxation of the shear components L_{13}^{micro} and L_{23}^{micro} for a cluster obtained after rolling (Lamel model) X1 = RD, X2 = TD, X3 = ND.

Consequently, we can write the velocity gradient of the two grains as a function of the macroscopic velocity gradient (Einstein's summation is applied on rlx index):

$$\begin{aligned} \underline{\underline{L}}^{micro,I} &= \underline{\underline{L}}^{Macro} + \dot{\gamma}^{rlx}\,\underline{\underline{L}}^{rlx} \\ \underline{\underline{L}}^{micro,II} &= \underline{\underline{L}}^{Macro} - \dot{\gamma}^{rlx}\,\underline{\underline{L}}^{rlx} \end{aligned} \tag{1}$$

The choice of the relaxation is justified by the fact that the Lamel model is also especially dedicated to rolling textures (with flattened and elongated grains). The relaxations considered in the cluster are represented in Figure 1.

It should be noticed that the chosen relaxations leave the rolling plane (X1 – X2) undistorted and not rotated (compared to the macroscopic deformation) and that equal and opposite shear stresses are imposed in each grain of the cluster (for each relaxation mode) to achieve a partial equilibrium and ensure a consistent interface. The stress equilibrium (concerning the relaxed components) is assured at the interface of the grains in the cluster without requiring that these shear stresses would be equal to zero as it is done in the classical relaxed-constraints models.

The Advanced Lamel model is an attempt to solve the problem of the grain shape. Its mathematical description only differs slightly from the Lamel model. In the Lamel model, the interfaces between two adjacent grains must always be parallel to the RD – TD plane. This constraint limits this model to rolling processes. In the recent Advanced Lamel (ALAMEL) model, the orientations of the interfaces are defined either by the user as a function of the material and the process investigated or they can be randomly chosen with a rule taking into account the grain shape. Therefore, the ALAMEL model is suitable for any deformation mode and different grain shapes (not only flat, elongated grains).

C_{11}[MPa]	C_{12}[MPa]	C_{13}[MPa]	C_{33}[MPa]	C_{44}[MPa]
16.24 10^4	9.2 10^4	6.9 10^4	18.07 10^4	4.67 10^4

Table 1: Elastic parameters of the Ti-α [3-4]

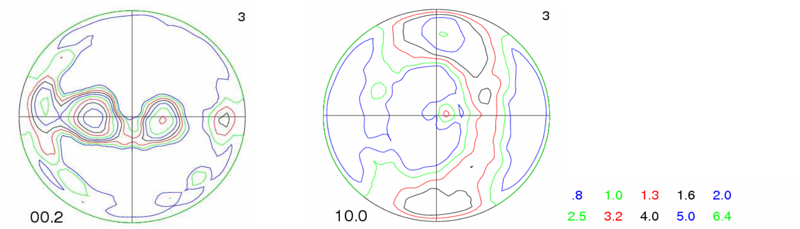

Figure 2: Texture of the Ti-α before deformation

3 MATERIAL AND EXERIMENTAL TESTS

The material used in this study is pure titanium having a main α phase (hexagonal crystal lattice). Its elastic moduli are presented in Table 1. The initial texture of the Ti-α is shown in Figure 2. Experimental simple shear tests along 0°, 45° and 90° from the rolling direction (RD) were performed on this material.

4 NUMERICAL RESULTS

4.1 Optimisation Procedure

Based on a previous sensitivity study of the critical resolved shear stresses (CRSS) influence on the behaviour of hexagonal closed packed (hcp) materials [5], an optimisation procedure on the hardening parameters was performed to fit the experimental results. A non linear optimisation algorithm (Generalized Reduced Gradient was used). The method is sketched in Figure 3, where τ_{C0}, Γ_0 and n are material parameters describing the evolution of the CRSS (τ_C) for all the slip systems as a function of the accumulated plastic slip (Γ_{tot}) according to Equation (2).

$$\tau_C = \tau_{C0}\left(1+\frac{\Gamma_{tot}}{\Gamma_0}\right)^n \tag{2}$$

The optimisation was performed on the simple shear test along RD (see Figure 4). The numerical results along 45° and 90° from RD were obtained using the MULTISITE model with the hardening parameters fitted along RD, i.e. $\tau_{C0} = 34.21\text{MPa}$, $\Gamma_0 = 0.096$ and $n = 0.1814$.

4.2 Results and discussions

Figure 4 presents the experimental results during simple shear tests along different direction from RD and the corresponding numerical predictions. As it was selected for the fitting procedure, the experimental and numerical curves along RD are effectively superimposed. The results at 90° from RD are in rather good agreement with the experiment, especially for large shear strains. Conversely the numerical prediction at 45° from RD is quite far from the experimental result. It should be noted that, for the present computations, the CRSS were obtained from a previous study [5] based on the material behaviour during simple tensile tests. Other CRSS values adapted to simple shear tests should be investigated to improve the numerical predictions with the crystal plasticity law.

A noticeable slope change in the hardening curves was obtained during the numerical shear simulations (particularly at 45° and 90° from RD), which could be attributed to texture evolution during shearing.

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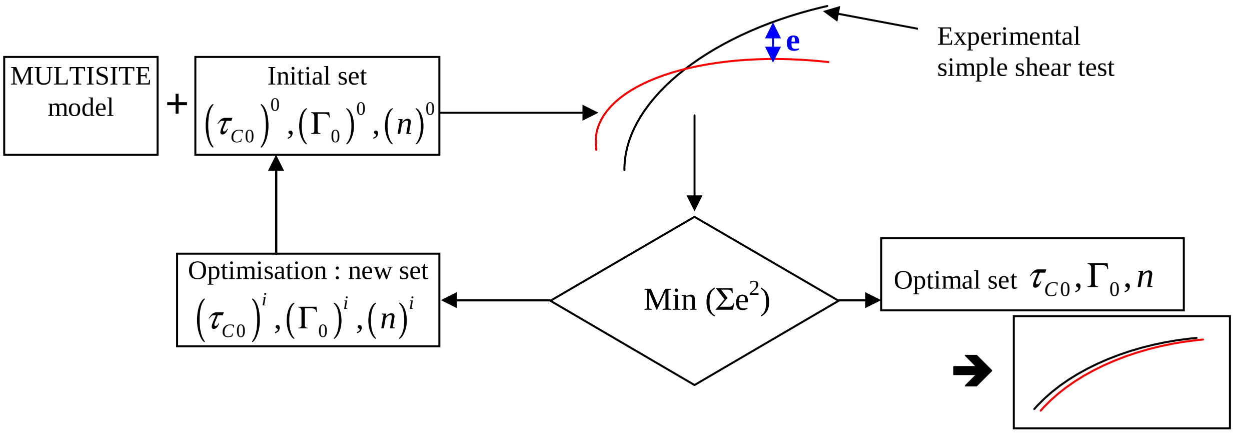

Figure 3: Optimisation procedure for the hardening parameters

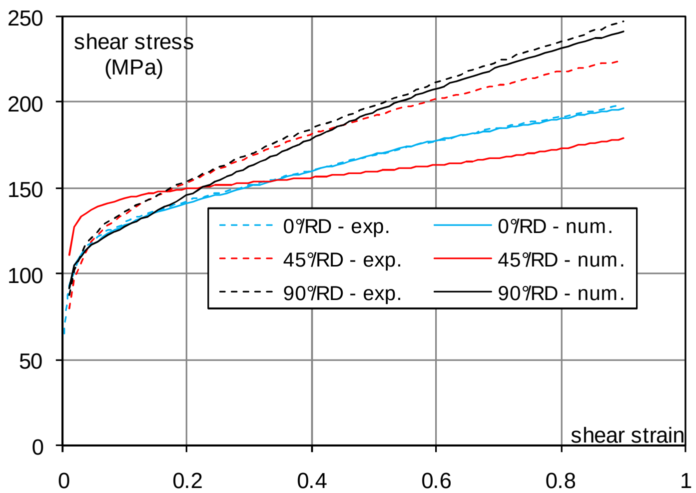

Figure 4: Mechanical behaviour during simple shear tests

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